Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 90.0 °C

Global applicability domain: Inside

Local applicability domain index: 6.21e-01

Confidence level: 7.55e-01

Nearest Neighbors from the Training Set

Image not found
Isopropanol
Measured: 82.3
Predicted: 90.0

Image not found
1-Propanol
Measured: 97.2
Predicted: 96.5

Image not found
Ethyl hydroperoxide
Measured: 95.0
Predicted: 99.9

Image not found
tert-Butyl alcohol
Measured: 82.4
Predicted: 97.0

Image not found
2-Chloroethanol
Measured: 129
Predicted: 122